

Hierarchical Random Telegraph Signals in Nano-junctions with Coulomb Correlations

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We propose a microscopic hamiltonian together with a master equation description to model stochastic hierarchical Random Telegraph Signal (RTS) or Pop-corn noise in nano-junctions. The microscopic model incorporates the crucial Coulomb correlations due to the trapped charges inside the junction or at the metal-oxide interface. The exact solution of the microscopic model is based on a generalization of the Nozières-De Dominicis method devised to treat the problem of the edge singularity in the X-ray absorption and emission spectra of metals. In the master equation description, the experimentally accessible transition rates are expressed in terms of the exact multi-channel Scattering matrix of the microscopic hamiltonian.

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In the last two decades, the experimental as well as the theoretical investigations of noise in sub-micron structures have developed into a new and fascinating subfield of mesoscopic physics [1]. Recently a resurgence of interest in tunneling through quantum dots and other nano-structures has taken place, presumably due to progress in the field of low-dimensional strongly correlated systems. As electronic devices are reduced to sub-micron sizes, stochastic fluctuations start to dominate their transport properties. In this letter we focus on generation-recombination noise that is often observed in semi-conductors and is interpreted as due to fluctuations in the number of carriers from the conduction (valence) band into traps in the band gap. Random Telegraph Signal noise (RTS) or Pop-corn noise is a special case of generation-recombination noise. The RTS may reflect the transition of single ions or trapped electrons between various meta-stable states inside the nano-structure.

Tunneling through charge defects at interfaces or junctions has been discussed in the literature earlier [2, 3]. In particular, Matveev and Larkin showed that the current-voltage characteristic of a tunnel-junction with a localized impurity level exhibits a power-law singularity due to Coulomb interactions between the charge carriers in the leads and the local charge impurity [4]. Remarkably enough, Geim et al. and Cobden and Muzykantskii measured the Fermi-edge singularity in resonant tunneling and in RTS noise [5, 6]. More recently Doudin et al. observed RTS fluctuations of up to 50% of the average magneto-resistance in ultra-small junctions [7]. Our investigations build further on these works. We do not discuss here the problem of dephasing as referred to in [8].

In this letter, we propose and solve a microscopic model as well as a phenomenological description of Pop-corn noise observed in tunneling through nano-junctions such as metal-oxide-metal nano-structures (extensions of this work to semi-conductor-oxide-semiconductor structures, etc. are possible). At fixed chemical potentials,

the current (conductance) jumps in a random yet hierarchical manner between discrete levels (see Figure 1). We argue that strong Coulomb correlations between trapped charges located inside the junction (or at the metal-oxide interface) and carriers in the leads govern the stochastic switching between the different values of the current (conductance). In the multi-channel and multi-trap case, we express the transition rates in a master equation description in terms of the parameters of the microscopic hamiltonian.

The model hamiltonian reads

$$\begin{aligned}
 H = & \sum_{jj'} \epsilon^{jj'} d_j^\dagger d_{j'} + \sum_{k\alpha} \epsilon_k^\alpha c_{k\alpha}^\dagger c_{k\alpha} \\
 & + \sum_{jj'} U^{jj'} d_j^\dagger d_j d_{j'}^\dagger d_{j'} \\
 & + \sum_{k\dots\alpha'} W_{kk'\alpha\alpha'}^0 c_{k\alpha}^\dagger c_{k'\alpha'} \\
 & + \sum_{k\dots\alpha'} W_{kk'\alpha\alpha'}^{jj'} c_{k\alpha}^\dagger c_{k'\alpha'} d_j^\dagger d_j \\
 & + \sum_{kj\alpha} \left(V_{k\alpha}^j c_{k\alpha}^\dagger d_j + h.c. \right)
 \end{aligned} \tag{1}$$

where $c_{k\alpha}^\dagger$ creates an electron of momentum k in lead $\alpha = L, R$; more generally the index α may also label the various transverse channels $\alpha = 1, \dots, n_c$ inside the leads. For simplicity's sake we shall omit here spin degrees of freedom. d_j^\dagger creates an electron in a localized state j inside the junction and at the interface. Traps can fluctuate in space between different meta-stable positions or migrate, yet we shall neglect these fluctuations. $\epsilon^{jj'}$ denotes the energy of and transfer between localized states. For simplicity, here we shall assume diagonal $\epsilon^{jj'} = \delta_{jj'} E_j$. ϵ_k^α denotes the conduction band energies and $\mu_\alpha = \epsilon_{k_F}^\alpha$ the chemical potential in channel α . Moreover ν_α is the density of states at the α Fermi level. $U^{jj'}$ denotes the Coulomb repulsion between localized states inside the junction. Because of its crucial role in the hierarchical structure of tunneling, we shall treat this term

at the mean-field level [9]. $W_{kk'\alpha\alpha'}^0$ represents the direct tunneling (non-diagonal matrix elements in the α indices) and backscattering (diagonal matrix elements) due to the metal-oxide interface. In the standard treatment of tunneling, only the non-diagonal part of this term is taken into account. The physical effect of the backscattering potential is a renormalization of the momentum (energy)-dependent effective density of states in the usual formula for the tunneling current. $W_{kk'\alpha\alpha'}^{jj'}$ denotes the Coulomb scattering between localized and extended states and represents the charge assisted tunneling. The terms $W_{kk'\alpha\alpha'}^0$ and $W_{kk'\alpha\alpha'}^{jj'}$ play a central role in this work and, should we emphasize, shall be treated exactly below. $V_{k\alpha}^j$ denotes the transfer integral between localized states inside the junction (or at the interface) and extended states in the leads.

To give a simple physical picture of the tunneling with trapping we consider an hydrodynamical description of the electron fluids in the leads. At wave-lengths that are much larger than the average spacing between the particles, the charge and magnetization density fluctuations are described by harmonic oscillators that can be quantized. Coulomb correlations within the leads in the charge and spin degrees of freedom are included in this semi-classical heuristic argument. As charge δQ and magnetization δM are being trapped in the junction (or at the interface), the electron fluids in the leads screen the accumulated charge and magnetization. After trapping has taken place, the energy increment consists in the charging and magnetizing terms proportional to δQ^2 , respectively, δM^2 , plus a Coulomb term between the charge and spin fluctuations in the leads and the local charge and magnetization in the junction (or at the interface): the charge and spin density fluctuations can be described by displaced harmonic oscillators. Hence the overlap between the de-trapped and the trapped configurations is a Gaussian in the charge and magnetization density fluctuations which vanishes in the infrared limit for Coulomb potential and one-dimensional longitudinal modes. In reality, the rate of charge $\delta \dot{Q}$ and magnetization $\delta \dot{M}$ accumulation in the junction is proportional to the charge and spin current density differentials between the (channels) right and left leads. As a result a dynamical cascade of Infrared Catastrophes occurs.

There are a number of experiments [2, 5, 6, 7] where the Markov property of the random switching process has been observed. Hence, we consider a description in real time in terms of a master equation. The idea is: i) to compute, for a fixed configuration \mathbf{a} of trapped carriers, the charge assisted tunneling current $\langle I \rangle_{\mathbf{a}}$ at fixed chemical potentials [9]. The configuration vector $\mathbf{a} = (a_1, \dots, a_N)$ refers to $a_j = 1$ if the local state $j = 1, \dots, N$ is occupied and $a_j = 0$ otherwise; ii) to evaluate the average current and the current-current correlation function through the junction by weighting each

configuration appropriately [9]. Subsequently we give expressions for the currents $\langle I \rangle_{\mathbf{a}}$ and the current-current correlation function.

Combining a projection technique with partial tracing of bath (channels) degrees of freedom [10], we arrive at a master equation for the diagonal matrix elements of the local density operator, i.e., for the probability density at time t of being in a configuration \mathbf{a} as

$$\dot{p}(\mathbf{a}, t) = -\hat{\lambda}^{\mathbf{a}} p(\mathbf{a}, t) + \sum_{\tilde{\mathbf{a}} \neq \mathbf{a}} \lambda_{\tilde{\mathbf{a}}}^{\mathbf{a}} p(\tilde{\mathbf{a}}, t) \quad , \quad \hat{\lambda}^{\mathbf{a}} = \sum_{\tilde{\mathbf{a}} \neq \mathbf{a}} \lambda_{\tilde{\mathbf{a}}}^{\mathbf{a}} \quad (2)$$

with the transition rates from \mathbf{a} to $\tilde{\mathbf{a}}$ given by

$$\lambda_{\tilde{\mathbf{a}}}^{\mathbf{a}} = 2\text{Re} \int_0^\infty dt \text{Tr}_B \left[\rho_{B\mathbf{a}}^{eq} \hat{H}'_{\tilde{\mathbf{a}}\mathbf{a}}(t) \hat{H}'_{\tilde{\mathbf{a}}\mathbf{a}}(0) \right] \quad (3)$$

where $\rho_{B\mathbf{a}}^{eq}$ represents the equilibrium density matrix for the bath (channels) with trap configuration \mathbf{a} . Notice that \mathbf{a} and $\tilde{\mathbf{a}}$ differ by a single site occupation. Further $\hat{H}'_{\tilde{\mathbf{a}}\mathbf{a}} = P_{\tilde{\mathbf{a}}} \hat{H}' P_{\mathbf{a}}$ denotes a projected interaction picture of the transfer term $H' = \sum_{k\alpha} \left(V_{k\alpha}^j c_{k\alpha}^\dagger d_j + h.c. \right)$. The Markov approximation underlying equation (2) requires the correlation time of the response function in equation (3) at finite temperature and in the presence of weak disorder to be much shorter than the characteristic time variations of the junction density matrix. For an arbitrary number of localized states the master equation (2) can be solved, in principle, by a method due to Kirchhoff [11]. A systematic Graph theoretic technique has also been developed by Weidlich [12]. Figure 1 illustrates a three level hierarchical RTS noise. The crucial point here is that the transition rates, which are experimentally accessible, can be expressed in terms of the local correlation function of the trapped states in the junction (or at the interface).

At this stage we have to tackle Dyson's equation for the transient propagator and from it infer the response function (3). To solve Dyson's equation a substantial generalization of a method developed by Nozières and De Dominicis in the context of the X-ray edge problem in metals [13, 14] is required. In the present case, Dyson's equation reduces to a system of singular integral equations that can be solved exactly by the techniques of Muskhelishvili and Vekua [9, 15, 16] (see also [19]). While the mathematics is rather involved let us attempt to explain in simple terms the essence of the method. We consider the process of single electron transfer into and off the trap state j_0 by H' , the occupation of all other localized states being fixed. The potential $W_{\mathbf{a}}$ acting on the conduction electrons can be written as the sum of all $W_{kk'}^j$ (considered as matrix in the indices $\alpha\alpha'$) for which $a_{j_0} = 1$ plus the direct tunneling and backscattering term $W_{kk'}^0$. A single electron transfer leads to $W_{\tilde{\mathbf{a}}}$, where $\tilde{\mathbf{a}}$ differs from \mathbf{a} by the occupation of the single site j_0 . Immediately after this single electron transfer the new potential felt by the conduction electrons reads $[W_{\tilde{\mathbf{a}}}^{\mathbf{a}}]_{kk'} = [W_{\tilde{\mathbf{a}}}]_{kk'} - [W_{\mathbf{a}}]_{kk'}$.

So the task can be decomposed into two steps, namely compute the propagator for a particle subject to the potential $W_{\mathbf{a}}$, and then extract the transient propagator for the potential $W_{\mathbf{a}}^{\mathbf{a}}$ which acts during a finite time interval. This transient propagator allows to obtain the response function required to compute the transition rate (3). Following Nozières and De Dominicis, we assume separable potentials $W_{kk'\alpha\alpha'}^0 = W_0^{\alpha\alpha'} u_{k\alpha} u_{k'\alpha'}$, $W_{kk'\alpha\alpha'}^{jj'} = \delta_{jj'} W_j^{\alpha\alpha'} u_{k\alpha} u_{k'\alpha'}$, and $V_{k\alpha}^j = V_{\alpha}^j u_{k\alpha}$ where $u_{k\alpha}$ is a cut-off function centered around the α Fermi surface, and take into account S-wave scattering only. This factorization simplifies the mathematics without affecting the physics, as it allows to perform readily the sums over k to obtain the local propagators at the junction. With these assumptions, the finite temperature transition rate for an arbitrary number of traps, including direct tunneling, reads

$$\lambda_{\mathbf{a}}^{\mathbf{a}} = 2\pi \operatorname{Re} \sum_{\alpha_1 \kappa} \left(\frac{i\xi_0 \beta}{2\pi} \right)^{\epsilon_{\alpha_1}} \times \frac{2\Gamma(\epsilon_{\alpha_1}) \mathcal{A}_{\alpha_1 \kappa}}{\left| \Gamma \left(\frac{\epsilon_{\alpha_1} + 1}{2} + i \frac{\beta}{2\pi} |\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\kappa}| \right) \right|^2} \times \frac{\cosh \left(\frac{\beta}{2} (\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\kappa}) - i \frac{\pi}{2} \epsilon_{\alpha_1} \right)}{\cosh(\beta(\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\kappa})) + \cos(\pi \epsilon_{\alpha_1})} \quad (4)$$

where ξ_0 is of the order of the conduction bandwidths, $\Gamma(x)$ denotes Euler's Gamma function and $\beta = 1/k_B T$ the inverse temperature. The $-$ sign refers to trapping (absorption) and the $+$ sign to de-trapping (emission). $\kappa = 1, \dots, m_c (\leq n_c)$ labels distinct chemical potentials μ_{κ} . $\tilde{E}_{\mathbf{a}}^{\mathbf{a}} = \tilde{E}_{\mathbf{a}} - \tilde{E}_{\mathbf{a}}$ with $\tilde{E}_{\mathbf{a}}$ being the energy of the localized state renormalized (closed loop contributions) by the potential $W_{\mathbf{a}}$, i.e., $\tilde{E}_{\mathbf{a}} = E_{\mathbf{a}} + \Delta E_{\mathbf{a}}^0 = \sum_{j=1}^N a_j E_j + \Delta E_{\mathbf{a}}^0$. The local Coulomb repulsion between trapped charges can be incorporated in the mean field approximation and contributes an additional term $U N_{\mathbf{a}}(N_{\mathbf{a}} - 1)/2$ to the energy $\tilde{E}_{\mathbf{a}}$, with $N_{\mathbf{a}}$ the number of trapped charges in configuration \mathbf{a} , and U the average potential in the junction. Furthermore $\mathcal{A}_{\alpha_1 \kappa}$ is given by

$$\mathcal{A}_{\alpha_1 \kappa} = -i \sum_{\alpha \alpha'} V_{\alpha}^{j_0} (D_{\mathbf{a}+}^{-1} D_{\mathbf{a}+} (B_{\mathbf{a}}^{\mathbf{a}})^{-1})_{\alpha \alpha_1} (B_{\mathbf{a}}^{\mathbf{a}} D_{\mathbf{a}+}^{-1} D_{\mathbf{a}+} \Lambda_{\kappa}^{\tilde{\mathbf{a}}})_{\alpha_1 \alpha'} V_{\alpha'}^{j_0} \quad (5)$$

where j_0 denotes the trap subject to the change in occupation number ($a_{j_0} \neq \tilde{a}_{j_0}$). $\nu_{\alpha\alpha'} = \nu_{\alpha} \delta_{\alpha\alpha'}$ is the density of states at the Fermi level μ_{α} and we have defined the matrices (assuming summation over $\hat{\alpha}$)

$$(D_{\mathbf{a}\pm})_{\alpha\alpha'} = [\pi(\tan \theta_{\alpha} \pm i) \nu_{\alpha}]^{-1} \delta_{\alpha\alpha'} + W_{\mathbf{a}}^{\alpha\alpha'} \quad (6)$$

$$\Lambda_{\kappa}^{\tilde{\mathbf{a}}} = [\Sigma_{\kappa}^{\tilde{\mathbf{a}}}]^{-1} \chi_{\kappa} \nu W_{\tilde{\mathbf{a}}} [\Sigma_{\kappa-1}^{\tilde{\mathbf{a}}}]^{-1} (\nu W_{\tilde{\mathbf{a}}})^{-1} \quad (7)$$

$$(\Sigma_{\kappa}^{\tilde{\mathbf{a}}})_{\alpha\alpha'} = \delta_{\alpha\alpha'} + \pi(\tan \theta_{\alpha} + i\sigma(\alpha, \kappa)) \nu_{\alpha} W_{\tilde{\mathbf{a}}}^{\alpha\alpha'} \quad (8)$$

with $\sigma(\alpha, \kappa) = +1$ if $\mu_{\alpha} < \mu_{\kappa}$ and -1 if $\mu_{\alpha} \geq \mu_{\kappa}$ and $(\chi_{\kappa})_{\alpha\alpha'} = \delta_{\alpha\alpha'} \delta_{\mu_{\alpha}, \mu_{\kappa}}$. We furthermore have assumed that $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n_c}$. The angle θ_{α} parameterizes the short time behavior of the single particle propagator in channel α [13]. The matrix $\mathcal{S}_{\mathbf{a}}^{\mathbf{a}} = D_{\mathbf{a}+}^{-1} D_{\mathbf{a}+} D_{\mathbf{a}-}^{-1} D_{\mathbf{a}-}$ is related to the generalized multi-channel Scattering matrices, $\mathcal{S}_{\mathbf{a}} = D_{\mathbf{a}+} D_{\mathbf{a}-}^{-1}$, and is diagonalized by $B_{\mathbf{a}}^{\mathbf{a}}$, $\mathcal{S}_{\mathbf{a}}^{\mathbf{a}} = B_{\mathbf{a}}^{\mathbf{a}} e^{2i\delta_{\mathbf{a}}^{\mathbf{a}}} (B_{\mathbf{a}}^{\mathbf{a}})^{-1}$, with the real eigenvalues $\delta_{\mathbf{a}}^{\mathbf{a}} = \operatorname{diag}((\delta_{\mathbf{a}}^{\mathbf{a}})_1, \dots, (\delta_{\mathbf{a}}^{\mathbf{a}})_{n_c})$. We use the notation $\epsilon_{\alpha_1} = \pm 2(\delta_{\mathbf{a}}^{\mathbf{a}})_{\alpha_1} / \pi - \operatorname{Tr}((\delta_{\mathbf{a}}^{\mathbf{a}})^2) / \pi^2$.

In the low temperature limit $k_B T \ll |\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\alpha_1}|$ the transition rates show the power-law divergence with the exponents ϵ_{α_1} known from the X-ray problem [13, 14]. The first correction in T is proportional to $(k_B T / |\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\kappa}|)^2$. In the high temperature limit, $k_B T \gg |\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \mp \mu_{\alpha_1}|$, λ shows a power-law behavior in T ,

$$\lambda_{\mathbf{a}}^{\mathbf{a}} \sim \sum T^{-\epsilon_{\alpha_1}}. \quad (9)$$

Specializing to a single trap, a single channel, and in the absence of direct tunneling the finite temperature expression (4) reduces to the result of [6] (their Eq. (5)). The effect of finite temperature is a broadening of the edge singularity, as illustrated in Figure 2. A similar broadening occurs in the case of weak disorder in weakly coupled electrodes: The exponential decay of the electron propagators in the electrodes leads to an imaginary contribution to the singular denominator, $|\tilde{E}_{\mathbf{a}}^{\mathbf{a}} \pm \mu_{\kappa} + i\gamma_{\alpha}|$, where $\gamma_{\alpha} = \pi \nu_{\alpha} n_{\text{dis}, \alpha} U_{\text{dis}, \alpha}^2$ and $n_{\text{dis}, \alpha}$, $U_{\text{dis}, \alpha}$ are the impurity density and the weak disorder potential in the channel α , respectively.

For a fixed configuration \mathbf{a} it is possible to adapt the method provided by Caroli et al. [3] to the calculation of the tunneling current in the presence of the backscattering $W_{\mathbf{a}}^{\alpha\alpha'} (\alpha \neq \alpha')$. The result for the simplest case of two channels $\alpha = L, R$ is given by

$$\langle I \rangle_{\mathbf{a}} = e \int \frac{d\omega}{2\pi} \frac{W_{\mathbf{a}}^{LR} \rho_L^h(\omega) \rho_R^e(\omega) - W_{\mathbf{a}}^{RL} \rho_R^h(\omega) \rho_L^e(\omega)}{\mathcal{D}^r(\omega) \mathcal{D}^a(\omega)}, \quad (10)$$

where e is the electron charge, $\rho_{\alpha}^h(\omega)$, $\rho_{\alpha}^e(\omega)$ represent the density of holes and electrons in the electrode α respectively, and

$$\mathcal{D}^{r,a}(\omega) = (1 - W_{\mathbf{a}}^{LL} g_L^{r,a}(\omega))(1 - W_{\mathbf{a}}^{RR} g_R^{r,a}(\omega)) - W_{\mathbf{a}}^{LR} W_{\mathbf{a}}^{RL} g_L^{r,a}(\omega) g_R^{r,a}(\omega), \quad (11)$$

with $g_{\alpha}^{r,a}$ the retarded and advanced free Green's functions in channel α . As an illustration for the current-current correlation function, $S_{II}(t)$, we choose a system with a single trap, $\mathbf{a} = a = 0, 1$. In the master equation approach S_{II} becomes

$$S_{II}(t) = e^{-(\lambda_1^0 + \lambda_0^0)|t|} \frac{\lambda_1^0 \lambda_0^0}{(\lambda_1^0 + \lambda_0^0)^2} (\langle I \rangle_1 - \langle I \rangle_0)^2. \quad (12)$$

In summary, we have been able to evaluate, for an arbitrary number of trapped charges, the transition rates of the master equation description of RTS noise and the tunneling current in terms of microscopic model hamiltonian parameters. We emphasize that this approach is not restricted to two-level systems which is often found in the literature [8], but allows for several fluctuators that can create a more complex, in particular an hierarchical, RTS noise. In future work, we intend to take into account the correlations in the leads (channels) as well as spin degrees of freedom. The latter are required, for example, to model RTS noise in magnetic nano-wires due to charge and magnetization trapping inside the junction.

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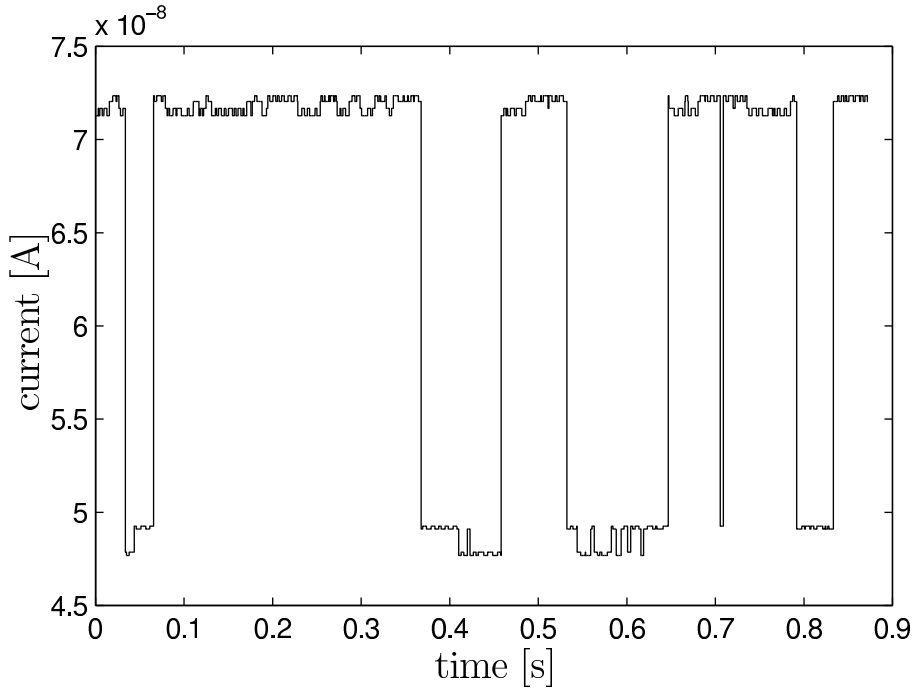


FIG. 1: Computation of a three-level RTS current fluctuations using Eqs. (4) and (10).

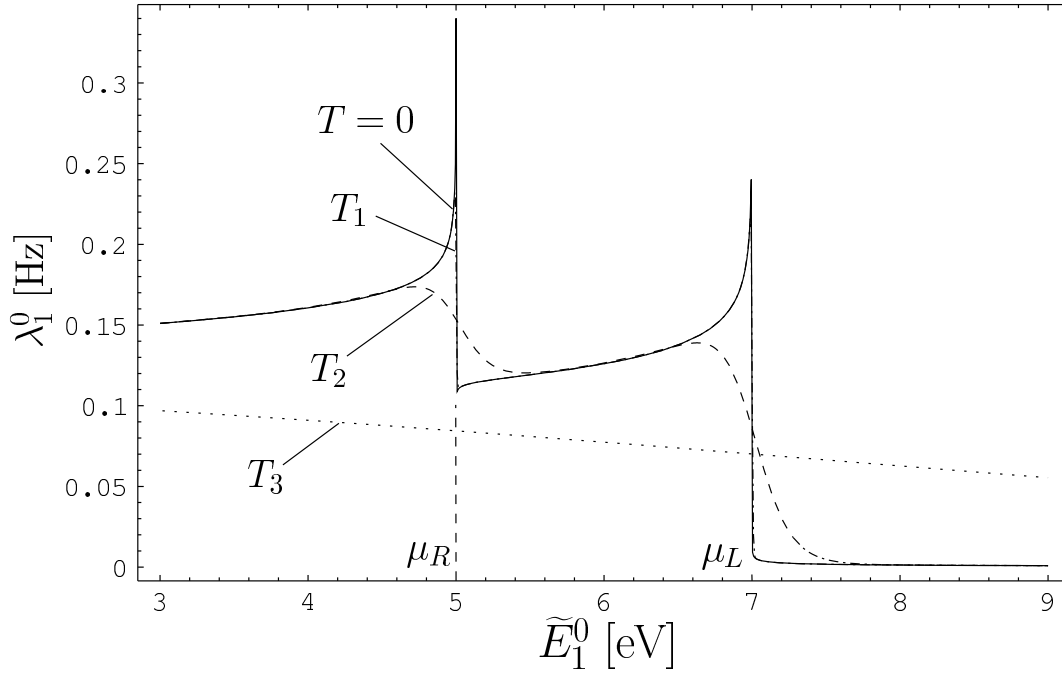


FIG. 2: Typical transition rate behavior in function of the energy of the localized state for the case of a single trap (Eq. (4)). The different curves correspond to the temperatures $T = 0, T_1 = T_3^{1/3} \approx 40$ K, $T_2 = T_3^{2/3} \approx 1500$ K, $T_3 = \mu_R/k_B \approx 60,000$ K.